

# AN ANALYSIS OF THE QUASI-NONLOCAL QUASICONTINUUM APPROXIMATION OF THE EMBEDDED ATOM MODEL

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**ABSTRACT.** The quasi-nonlocal quasicontinuum method (QNL) is a consistent hybrid coupling method for atomistic and continuum models. Embedded atom models are empirical many-body potentials that are widely used for FCC metals such as copper and aluminum. In this paper, we consider the QNL method for EAM potentials, and we give a stability and error analysis for a chain with next-nearest neighbor interactions. We identify conditions for the pair potential, electron density function, and embedding function so that the lattice stability of the atomistic and the EAM-QNL models are asymptotically equal.

## 1. INTRODUCTION

Hybrid atomistic-to-continuum methods couple atomistic regions surrounding defects with continuum regions to achieve the accuracy of the atomistic model and the efficiency of the continuum model. Quasicontinuum hybrid methods utilize the Cauchy–Born rule for the energy density in the continuum region [21]. The original quasicontinuum energy [21] (denoted QCE) has interfacial forces (called “ghost forces”) for a uniform strain [4, 24]. Thus, uniform strain is not an equilibrium solution for the QCE energy (even though uniform strain is an equilibrium for purely atomistic and for purely coarse-grained continuum models).

More accurate atomistic-to-continuum coupling methods have been proposed to remedy the QCE model. The ghost force correction method (GFC) achieves an increased accuracy by adding a correction to the ghost forces as a dead load during a quasistatic process [4, 5, 10, 18, 24]. The GFC method can be viewed as a stationary iterative method [4, 5, 10, 18] to solve the force-based quasicontinuum approximation (QCF) using QCE as a preconditioner. More accurate coupling can be achieved by using a more accurate preconditioner or by using GMRES acceleration to solve the QCF equilibrium equations [3, 7, 8, 17], but the non-conservative and indefinite QCF equilibrium equations make the iterative solution and the determination of lattice stability more challenging [10].

An alternative approach is to develop a quasicontinuum energy that is more accurate than QCE. We will call a QC energy *consistent* if it does not have ghost forces for a uniformly strained lattice. The quasi-nonlocal energy (QNL) was the first consistent quasicontinuum energy [25]. For a one dimensional chain, the original QNL method is restricted to next-nearest neighbor interactions [25]. The QNL method for pair interaction potentials was extended to finite range interactions in [15] and to two dimensional finite range problems in [23].

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In this paper, we formulate a one-dimensional QNL energy for the embedded atom model (EAM) following [25]. The embedded atom model [12, 14, 20] is an empirical many-body potential that is widely used to model FCC metals such as copper and aluminum. We then give an analysis of the stability and error for the EAM-QNL approximation in the next-nearest neighbor case for a periodic chain.

We identify conditions for the pair potential, electron density function, and embedding function so that the lattice stability of the atomistic and the EAM-QNL models are asymptotically equal. We also show in Remark 4.4 that the atomistic and EAM-QNL models can be less stable than the local quasicontinuum model (EAM-QCL), which is the EAM-QNL model with no atomistic region, if the above conditions on the pair potential, electron density function, and embedding function are not satisfied.

Many theoretical analyses of QC models have been given based on pair-potential interactions [1, 6, 9, 11, 15, 16, 19]. In this paper, we give an analysis of the stability and accuracy of a linearization of the quasi-nonlocal method for the EAM potential in one dimension with next-nearest neighbor interactions. A nonlinear *a priori* and *a posteriori* error analysis for the QNL model with next-nearest-neighbor pair potential interaction in one dimension was given in [22]. We think that a similar nonlinear analysis using the inverse function theorem can be done for this model, but we restrict our presentation in this paper to the linear analysis for simplicity.

In Section 2, we present the notation used in this paper. We define the displacement space  $\mathcal{U}$  and the deformation space  $\mathcal{Y}_F$ . We then introduce the norms we will use to estimate the modeling error and the displacement gradient error. In Section 3, we introduce the QNL model with next-nearest neighbor interaction for the EAM potential.

In Section 4, we give sharp stability estimates for both the fully atomistic model and the EAM-QNL model for a uniformly strained chain. Sharp stability estimates are necessary to determine whether quasicontinuum methods (or other coupling methods) are accurate near instabilities such as defect formation or crack propagation [7, 9]. Similar stability estimates for the fully atomistic and fully local quasi-continuum (QCL) models can also be obtained by discrete Fourier analysis [13].

In section 5, we study the convergence rate of the EAM-QNL model. We compare the equilibrium solution of the EAM-QNL model with that of the fully atomistic model, and we use the negative norm estimation method [8, 15] to obtain an optimal rate of convergence of the strain error. The error estimate depends only on the smoothness of the strain in the continuum region and holds near lattice instabilities, thus demonstrating that the QNL method for the EAM potential can give a small error if defects are captured in the atomistic region.

## 2. NOTATION

In this section, we present the notation used in this paper. We define the scaled reference lattice

$$\epsilon\mathbb{Z} := \{\epsilon\ell : \ell \in \mathbb{Z}\},$$

where  $\epsilon > 0$  scales the reference atomic spacing and  $\mathbb{Z}$  is the set of integers. We then deform the reference lattice  $\epsilon\mathbb{Z}$  uniformly into the lattice

$$F\epsilon\mathbb{Z} := \{F\epsilon\ell : \ell \in \mathbb{Z}\}$$

where  $F > 0$  is the macroscopic deformation gradient, and we define the corresponding deformation  $\mathbf{y}_F$  by

$$(\mathbf{y}_F)_\ell := F\epsilon\ell \quad \text{for } -\infty < \ell < \infty.$$

For simplicity, we consider the space  $\mathcal{U}$  of  $2N$ -periodic zero mean displacements  $\mathbf{u} = (u_\ell)_{\ell \in \mathbb{Z}}$  from  $\mathbf{y}_F$  given by

$$\mathcal{U} := \left\{ \mathbf{u} : u_{\ell+2N} = u_\ell \text{ for } \ell \in \mathbb{Z}, \text{ and } \sum_{\ell=-N+1}^N u_\ell = 0 \right\},$$

and we thus admit deformations  $\mathbf{y}$  from the space

$$\mathcal{Y}_F := \{ \mathbf{y} : \mathbf{y} = \mathbf{y}_F + \mathbf{u} \text{ for some } \mathbf{u} \in \mathcal{U} \}.$$

We set  $\epsilon = 1/N$  throughout so that the reference length of the periodic domain is fixed.

We define the discrete differentiation operator,  $D\mathbf{u}$ , on periodic displacements by

$$(D\mathbf{u})_\ell := \frac{u_\ell - u_{\ell-1}}{\epsilon}, \quad -\infty < \ell < \infty.$$

We note that  $(D\mathbf{u})_\ell$  is also  $2N$ -periodic in  $\ell$  and satisfies the zero mean condition. We will denote  $(D\mathbf{u})_\ell$  by  $Du_\ell$ . We then define

$$\left( D^{(2)}\mathbf{u} \right)_\ell := \frac{Du_\ell - Du_{\ell-1}}{\epsilon}, \quad -\infty < \ell < \infty,$$

and we define  $(D^{(3)}\mathbf{u})_\ell$  and  $(D^{(4)}\mathbf{u})_\ell$  in a similar way. To make the formulas concise and more readable, we sometimes denote  $Du_\ell$  by  $u'_\ell$ ,  $D^{(2)}u_\ell$  by  $u''_\ell$ , etc., when there is no confusion in the expressions.

For a displacement  $\mathbf{u} \in \mathcal{U}$  and its discrete derivatives, we define the discrete  $\ell_\epsilon^2$  norms by

$$\|\mathbf{u}\|_{\ell_\epsilon^2} := \left( \epsilon \sum_{\ell=-N+1}^N |u_\ell|^2 \right)^{1/2}, \quad \|\mathbf{u}'\|_{\ell_\epsilon^2} := \left( \epsilon \sum_{\ell=-N+1}^N |u'_\ell|^2 \right)^{1/2}, \text{ etc.}$$

Finally, for smooth real-valued functions  $\mathcal{E}(\mathbf{y})$  defined for  $\mathbf{y} \in \mathcal{Y}_F$ , we define the first and second derivatives (variations) by

$$\begin{aligned} \langle \delta \mathcal{E}(\mathbf{y}), \mathbf{w} \rangle &:= \sum_{\ell=-N+1}^N \frac{\partial \mathcal{E}}{\partial y_\ell}(\mathbf{y}) w_\ell \quad \text{for all } \mathbf{w} \in \mathcal{U} \\ \langle \delta^2 \mathcal{E}(\mathbf{y}) \mathbf{v}, \mathbf{w} \rangle &:= \sum_{\ell, m=-N+1}^N \frac{\partial^2 \mathcal{E}}{\partial y_\ell \partial y_m}(\mathbf{y}) v_\ell w_m \quad \text{for all } \mathbf{v}, \mathbf{w} \in \mathcal{U}. \end{aligned}$$

### 3. THE EMBEDDED ATOM MODEL AND ITS QNL APPROXIMATION

We first give a description of the next-nearest neighbor EAM Model.

**3.1. The Next-Nearest-Neighbor Embedded Atom Model.** The total energy per period of the next-nearest neighbor EAM model is

$$\mathcal{E}_{tot}^a(\mathbf{y}) := \mathcal{E}^a(\mathbf{y}) + \mathcal{F}(\mathbf{y}) \tag{3.1}$$

for deformations  $\mathbf{y} \in \mathcal{Y}_F$  where  $\mathcal{E}^a(\mathbf{y})$  is the total atomistic energy and  $\mathcal{F}(\mathbf{y})$  is the total external potential energy. The total atomistic energy is the sum of the *embedding energy*,  $\hat{\mathcal{E}}^a(\mathbf{y})$ , and the *pair potential energy*,  $\tilde{\mathcal{E}}^a(\mathbf{y})$ :

$$\mathcal{E}^a(\mathbf{y}) := \hat{\mathcal{E}}^a(\mathbf{y}) + \tilde{\mathcal{E}}^a(\mathbf{y}). \tag{3.2}$$

The embedding energy is

$$\hat{\mathcal{E}}^a(\mathbf{y}) := \epsilon \sum_{\ell=-N+1}^N G(\bar{\rho}_\ell^a(\mathbf{y}))$$

where  $G(\bar{\rho})$  is the embedding energy function, the total electron density  $\bar{\rho}_\ell^a(\mathbf{y})$  at atom  $\ell$  is

$$\bar{\rho}_\ell^a(\mathbf{y}) := \rho(y'_\ell) + \rho(y'_\ell + y'_{\ell-1}) + \rho(y'_{\ell+1}) + \rho(y'_{\ell+1} + y'_{\ell+2}),$$

and  $\rho(r/\epsilon)$  is the electron density contributed by an atom at distance  $r$ . The pair potential energy is

$$\tilde{\mathcal{E}}^a(\mathbf{y}) := \epsilon \sum_{\ell=-N+1}^N \frac{1}{2} [\phi(y'_\ell) + \phi(y'_\ell + y'_{\ell-1}) + \phi(y'_{\ell+1}) + \phi(y'_{\ell+1} + y'_{\ell+2})]$$

where  $\epsilon\phi(r/\epsilon)$  is the pair potential interaction energy [12]. Our formulation allows general nonlinear external potential energies  $\mathcal{F}(\mathbf{y})$  defined for  $\mathbf{y} \in \mathcal{Y}_F$ , but we note that the total external potential energy for periodic dead loads  $\mathbf{f}$  is given by

$$\mathcal{F}(\mathbf{y}) := - \sum_{\ell=-N+1}^N \epsilon f_\ell y_\ell.$$

The equilibrium solution  $\mathbf{y}^a$  of the EAM atomistic model (3.1) then satisfies

$$-\langle \delta \mathcal{E}^a(\mathbf{y}^a), \mathbf{w} \rangle = -\langle \delta \hat{\mathcal{E}}^a(\mathbf{y}^a), \mathbf{w} \rangle - \langle \delta \tilde{\mathcal{E}}^a(\mathbf{y}^a), \mathbf{w} \rangle = \langle \delta \mathcal{F}(\mathbf{y}^a), \mathbf{w} \rangle \quad \text{for all } \mathbf{w} \in \mathcal{U}. \quad (3.3)$$

Here the negative of the embedding force of (3.3) is given by

$$\begin{aligned} \langle \delta \hat{\mathcal{E}}^a(\mathbf{y}^a), \mathbf{w} \rangle = & \epsilon \sum_{\ell=-N+1}^N G'(\bar{\rho}_\ell^a(\mathbf{y}^a)) \cdot \left[ \rho'(Dy_\ell^a)w'_\ell + \rho'(Dy_\ell^a + Dy_{\ell-1}^a)(w'_\ell + w'_{\ell-1}) \right. \\ & \left. + \rho'(Dy_{\ell+1}^a)w'_{\ell+1} + \rho'(Dy_{\ell+1}^a + Dy_{\ell+2}^a)(w'_{\ell+1} + w'_{\ell+2}) \right], \end{aligned}$$

the negative of the pair potential force of (3.3) is given by

$$\begin{aligned} \langle \delta \tilde{\mathcal{E}}^a(\mathbf{y}^a), \mathbf{w} \rangle = & \epsilon \sum_{\ell=-N+1}^N \frac{1}{2} \left[ \phi'(Dy_\ell^a)w'_\ell + \phi'(Dy_\ell^a + Dy_{\ell-1}^a)(w'_\ell + w'_{\ell-1}) \right. \\ & \left. + \phi'(Dy_{\ell+1}^a)w'_{\ell+1} + \phi'(Dy_{\ell+1}^a + Dy_{\ell+2}^a)(w'_{\ell+1} + w'_{\ell+2}) \right] \end{aligned}$$

and the external force is given by

$$\langle \delta \mathcal{F}(\mathbf{y}), \mathbf{w} \rangle = \sum_{\ell=-N+1}^N \frac{\partial \mathcal{F}}{\partial y_\ell}(\mathbf{y}) w_\ell \quad \text{for all } \mathbf{w} \in \mathcal{U}.$$

### 3.2. The Quasi-Nonlocal EAM Approximation for Next-Nearest-Neighbor Interactions.

Hybrid atomistic-to-continuum methods can give an accurate and efficient solution if the deformation  $\mathbf{y} \in \mathcal{Y}_F$  is "smooth" in most of the computational domain, but not in the remaining domain where defects occur [8, 22]. The goal of QC methods is to decompose the reference lattice into an atomistic region with defects and a continuum region with long-range elastic effects. It applies an atomistic model to the atomistic region for accuracy and a continuum model to the continuum region for efficiency.

In this paper, we will consider an atomistic region defined by the atoms with reference positions  $x_\ell$  for  $\ell = -K, \dots, K$ , and a continuum region for  $\ell \in \{-N+1, \dots, -(K+3)\} \cup \{(K+3), \dots, N\}$ . To

eliminate the ghost force that energy-based quasicontinuum approximations can have [6, 17, 21, 25], we define the remaining atoms,  $\pm(K+1), \pm(K+2)$ , to be quasi-nonlocal atoms [6, 25]. For the pair potential energy, the quasi-nonlocal atoms  $\pm(K+1), \pm(K+2)$  interact without approximation with atoms in the atomistic region, but interact through the continuum Cauchy-Born approximation with all other atoms [25]. The interactions of the quasi-nonlocal atoms for the embedding energy is slightly more complex, as given in [25] and below.

The atomistic energy associated with each atom is given by

$$\mathcal{E}_\ell^a(\mathbf{y}) := \hat{\mathcal{E}}_\ell^a(\mathbf{y}) + \tilde{\mathcal{E}}_\ell^a(\mathbf{y}) = G(\bar{\rho}_\ell^a(\mathbf{y})) + \frac{1}{2} [\phi(y'_\ell) + \phi(y'_\ell + y'_{\ell-1}) + \phi(y'_{\ell+1}) + \phi(y'_{\ell+1} + y'_{\ell+2})]$$

where  $\hat{\mathcal{E}}_\ell^a(\mathbf{y})$  denotes the embedding energy at atom  $\ell$  and  $\tilde{\mathcal{E}}_\ell^a(\mathbf{y})$  denotes the pair potential energy at atom  $\ell$  ( $\hat{\mathcal{E}}_\ell^c(\mathbf{y})$ ,  $\hat{\mathcal{E}}_\ell^{qnl}(\mathbf{y})$ ,  $\tilde{\mathcal{E}}_\ell^c(\mathbf{y})$  and  $\tilde{\mathcal{E}}_\ell^{qnl}(\mathbf{y})$  will be defined analogously below), and the continuum energy associated with each atom is given by

$$\begin{aligned} \mathcal{E}_\ell^c(\mathbf{y}) := \hat{\mathcal{E}}_\ell^c(\mathbf{y}) + \tilde{\mathcal{E}}_\ell^c(\mathbf{y}) &= \frac{1}{2} G(\bar{\rho}_\ell^c(\mathbf{y})) + \frac{1}{2} G(\bar{\rho}_{\ell+1}^c(\mathbf{y})) \\ &\quad + \frac{1}{2} [\phi(y'_\ell) + \phi(2y'_\ell) + \phi(y'_{\ell+1}) + \phi(2y'_{\ell+1})] \end{aligned}$$

where the total continuum electron density at atom  $\ell$  is

$$\bar{\rho}_\ell^c(\mathbf{y}) := 2\rho(y'_\ell) + 2\rho(2y'_\ell).$$

To define the QNL energy for the quasi-nonlocal atoms, we define the QNL electron density at atom  $\ell$  by

$$\bar{\rho}_\ell^{qnl}(\mathbf{y}) := 2\rho(y'_\ell) + 2\rho(y'_\ell + y'_{\ell-1}).$$

We then define the QNL energy for the quasi-nonlocal atoms by

$$\begin{aligned} \mathcal{E}_{K+1}^{qnl}(\mathbf{y}) &:= \hat{\mathcal{E}}_{K+1}^{qnl}(\mathbf{y}) + \tilde{\mathcal{E}}_{K+1}^{qnl}(\mathbf{y}) \\ &= \frac{1}{2} G(\bar{\rho}_{K+1}^{qnl}(\mathbf{y})) + \frac{1}{2} G(\bar{\rho}_{K+2}^c(\mathbf{y})) \\ &\quad + \frac{1}{2} [\phi(y'_{K+1}) + \phi(y'_{K+2}) + \phi(y'_{K+1} + y'_K) + \phi(2y'_{K+2})] \end{aligned}$$

and

$$\begin{aligned} \mathcal{E}_{K+2}^{qnl}(\mathbf{y}) &:= \hat{\mathcal{E}}_{K+2}^{qnl}(\mathbf{y}) + \tilde{\mathcal{E}}_{K+2}^{qnl}(\mathbf{y}) \\ &= \frac{1}{2} G(\bar{\rho}_{K+2}^{qnl}(\mathbf{y})) + \frac{1}{2} G(\bar{\rho}_{K+3}^c(\mathbf{y})) \\ &\quad + \frac{1}{2} [\phi(y'_{K+2}) + \phi(y'_{K+3}) + \phi(y'_{K+2} + y'_{K+1}) + \phi(2y'_{K+3})]. \end{aligned}$$

We define the QNL energy in a symmetric way and so only give the formulas for  $0 \leq \ell \leq N$ .

The total energy per period of the QNL model is then given by

$$\begin{aligned} \mathcal{E}_{tot}^{qnl}(\mathbf{y}) &:= \epsilon \sum_{\ell=-N+1}^N \mathcal{E}_\ell^{qnl}(\mathbf{y}) + \mathcal{F}(\mathbf{y}) \\ &= \mathcal{E}^{qnl}(\mathbf{y}) + \mathcal{F}(\mathbf{y}) = \hat{\mathcal{E}}^{qnl}(\mathbf{y}) + \tilde{\mathcal{E}}^{qnl}(\mathbf{y}) + \mathcal{F}(\mathbf{y}), \end{aligned} \tag{3.4}$$

where

$$\mathcal{E}_\ell^{qnl}(\mathbf{y}) := \begin{cases} \mathcal{E}_\ell^a(\mathbf{y}) & \text{for } 0 \leq \ell < K+1, \\ \mathcal{E}_\ell^{qnl}(\mathbf{y}) & \text{for } \ell = K+1, K+2, \\ \mathcal{E}_\ell^c(\mathbf{y}) & \text{for } K+2 < \ell < N. \end{cases}$$

The equilibrium solution  $\mathbf{y}^{qnl}$  of the EAM-QNL model (3.4) then satisfies

$$-\langle \delta \mathcal{E}^{qnl}(\mathbf{y}^{qnl}), \mathbf{w} \rangle = -\langle \delta \hat{\mathcal{E}}^{qnl}(\mathbf{y}^{qnl}), \mathbf{w} \rangle - \langle \delta \tilde{\mathcal{E}}^{qnl}(\mathbf{y}^{qnl}), \mathbf{w} \rangle = \langle \delta \mathcal{F}(\mathbf{y}^{qnl}), \mathbf{w} \rangle \quad \text{for all } \mathbf{w} \in \mathcal{U}, \quad (3.5)$$

where the negative of the embedding force is given by

$$\begin{aligned} \langle \delta \hat{\mathcal{E}}^{qnl}(\mathbf{y}^{qnl}), \mathbf{w} \rangle = & \dots \\ & + \epsilon \sum_{\ell=0}^K G'(\bar{\rho}_\ell^a(\mathbf{y}^{qnl})) \cdot \left[ \rho'(Dy_\ell^{qnl})w'_\ell + \rho'(Dy_\ell^{qnl} + Dy_{\ell-1}^{qnl})(w'_\ell + w'_{\ell-1}) \right. \\ & \quad \left. + \rho'(Dy_{\ell+1}^{qnl})w'_{\ell+1} + \rho'(Dy_{\ell+1}^{qnl} + Dy_{\ell+2}^{qnl})(w'_{\ell+1} + w'_{\ell+2}) \right] \\ & + \epsilon G'(\bar{\rho}_{K+1}^{qnl}(\mathbf{y}^{qnl})) \cdot \left[ \rho'(Dy_{K+1}^{qnl})w'_{K+1} + \rho'(Dy_{K+1}^{qnl} + Dy_K^{qnl})(w'_{K+1} + w'_K) \right] \\ & + \epsilon G'(\bar{\rho}_{K+2}^c(\mathbf{y}^{qnl})) \cdot \left[ \rho'(Dy_{K+2}^{qnl})w'_{K+2} + 2\rho'(2Dy_{K+2}^{qnl})(w'_{K+2}) \right] \\ & + \epsilon G'(\bar{\rho}_{K+2}^{qnl}(\mathbf{y}^{qnl})) \cdot \left[ \rho'(Dy_{K+2}^{qnl})w'_{K+2} + \rho'(Dy_{K+2}^{qnl} + Dy_{K+1}^{qnl})(w'_{K+2} + w'_{K+1}) \right] \\ & + \epsilon G'(\bar{\rho}_{K+3}^c(\mathbf{y}^{qnl})) \cdot \left[ \rho'(Dy_{K+3}^{qnl})w'_{K+3} + 2\rho'(2Dy_{K+3}^{qnl})(w'_{K+3}) \right] \\ & + \epsilon \sum_{\ell=K+3}^N \left\{ G'(\bar{\rho}_\ell^c(\mathbf{y}^{qnl})) \cdot \left[ \rho'(Dy_\ell^{qnl})w'_\ell + 2\rho'(2Dy_\ell^{qnl})(w'_\ell) \right] \right. \\ & \quad \left. + G'(\bar{\rho}_{\ell+1}^c(\mathbf{y}^{qnl})) \cdot \left[ \rho'(Dy_{\ell+1}^{qnl})w'_{\ell+1} + 2\rho'(2Dy_{\ell+1}^{qnl})(w'_{\ell+1}) \right] \right\}, \end{aligned} \quad (3.6)$$

and the negative of the pair potential force is given by

$$\begin{aligned} \langle \delta \tilde{\mathcal{E}}^{qnl}(\mathbf{y}^{qnl}), \mathbf{w} \rangle = & \dots \\ & + \epsilon \sum_{\ell=0}^K \frac{1}{2} \left[ \phi'(Dy_\ell^{qnl})w'_\ell + \phi'(Dy_\ell^{qnl} + Dy_{\ell-1}^{qnl})(w'_\ell + w'_{\ell-1}) \right. \\ & \quad \left. + \phi'(Dy_{\ell+1}^{qnl})w'_{\ell+1} + \phi'(Dy_{\ell+1}^{qnl} + Dy_{\ell+2}^{qnl})(w'_{\ell+1} + w'_{\ell+2}) \right] \\ & + \frac{\epsilon}{2} \left[ \phi'(Dy_{K+1}^{qnl})w'_{K+1} + \phi'(Dy_{K+1}^{qnl} + Dy_K^{qnl})(w'_{K+1} + w'_K) \right] \\ & + \frac{\epsilon}{2} \left[ \phi'(Dy_{K+2}^{qnl})w'_{K+2} + 2\phi'(2Dy_{K+2}^{qnl})(w'_{K+2}) \right] \\ & + \frac{\epsilon}{2} \left[ \phi'(Dy_{K+2}^{qnl})w'_{K+2} + \phi'(Dy_{K+2}^{qnl} + Dy_{K+1}^{qnl})(w'_{K+2} + w'_{K+1}) \right] \\ & + \frac{\epsilon}{2} \left[ \phi'(Dy_{K+3}^{qnl})w'_{K+3} + 2\phi'(2Dy_{K+3}^{qnl})(w'_{K+3}) \right] \\ & + \epsilon \sum_{\ell=K+3}^N \frac{1}{2} \left[ \phi'(Dy_\ell^{qnl})w'_\ell + 2\phi'(2Dy_\ell^{qnl})w'_\ell + \phi'(Dy_{\ell+1}^{qnl})w'_{\ell+1} + 2\phi'(2Dy_{\ell+1}^{qnl})w'_{\ell+1} \right]. \end{aligned} \quad (3.7)$$

## 4. STABILITY ANALYSIS OF THE ATOMISTIC AND EAM-QNL MODELS

In this section, we will give a stability analysis for the atomistic model and the EAM-QNL model for the next-nearest neighbor case. We will use techniques similar to those presented in [9] for the atomistic and QNL method for pair potentials.

**4.1. The Atomistic Model.** The uniform deformation  $\mathbf{y}_F$  is an equilibrium of the atomistic model (3.2), therefore, we say that the equilibrium  $\mathbf{y}_F$  is stable in the atomistic model if and only if  $\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  is positive definite, that is,

$$\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle = \langle \delta^2 \hat{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle + \langle \delta^2 \tilde{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle > 0 \quad \text{for all } \mathbf{u} \in \mathcal{U} \setminus \{\mathbf{0}\}. \quad (4.1)$$

Note that  $\langle \delta^2 \tilde{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  is given by formula (7) in [9]:

$$\langle \delta^2 \tilde{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle = \tilde{A}_F \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 - \epsilon^2 \phi_{2F}'' \|D^{(2)}\mathbf{u}\|_{\ell_\epsilon^2}^2, \quad (4.2)$$

where

$$\tilde{A}_F := \phi_F'' + 4\phi_{2F}'' \quad \text{for} \quad \phi_F'' := \phi''(F) \quad \text{and} \quad \phi_{2F}'' := \phi''(2F) \quad (4.3)$$

is the *continuum elastic modulus for the pair interaction potential*. Thus, we only need to focus on  $\langle \delta^2 \hat{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$ , that is,

$$\begin{aligned} \langle \delta^2 \hat{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle = \epsilon \sum_{\ell=-N+1}^N \Big\{ & G_F'' [\rho_F'(u'_\ell + u'_{\ell+1}) + \rho_{2F}'(u'_{\ell-1} + u'_\ell + u'_{\ell+1} + u'_{\ell+2})]^2 \\ & + G_F' [\rho_F''(u'_\ell)^2 + \rho_{2F}''(u'_\ell + u'_{\ell-1})^2 + \rho_F''(u'_{\ell+1})^2 \\ & + \rho_{2F}''(u'_{\ell+1} + u'_{\ell+2})^2] \Big\}, \end{aligned} \quad (4.4)$$

where

$$\begin{aligned} \rho_F' &:= \rho'(F), \quad \rho_F'' := \rho''(F), \quad \rho_{2F}' := \rho'(2F), \quad \rho_{2F}'' := \rho''(2F), \\ G_F' &:= G'(\bar{\rho}_\ell^a(\mathbf{y}_F)) = G'(\bar{\rho}_\ell^c(\mathbf{y}_F)) = G'(\bar{\rho}_\ell^{qnl}(\mathbf{y}_F)), \\ G_F'' &:= G''(\bar{\rho}_\ell^a(\mathbf{y}_F)) = G''(\bar{\rho}_\ell^c(\mathbf{y}_F)) = G''(\bar{\rho}_\ell^{qnl}(\mathbf{y}_F)). \end{aligned}$$

We calculate the identities

$$\begin{aligned} (u'_\ell + u'_{\ell+1})^2 &= 2(u'_\ell)^2 + 2(u'_{\ell+1})^2 - \epsilon^2(u''_{\ell+1})^2, \\ (u'_\ell + u'_{\ell+1} + u'_{\ell+2})^2 &= 3(u'_\ell)^2 + 3(u'_{\ell+1})^2 + 3(u'_{\ell+2})^2 - 3\epsilon^2(u''_{\ell+1})^2 - 3\epsilon^2(u''_{\ell+2})^2 + \epsilon^4(u_{\ell+2}^{(3)})^2. \\ 2(u'_\ell + u'_{\ell+1}) \cdot (u'_{\ell-1} + u'_\ell + u'_{\ell+1} + u'_{\ell+2}) &= 2[(u'_{\ell-1})^2 + 3(u'_\ell)^2 + 3(u'_{\ell+1})^2 + (u'_{\ell+2})^2] \\ &\quad - 3\epsilon^2[(u''_\ell)^2 + 2(u''_{\ell+1})^2 + (u''_{\ell+2})^2] + \epsilon^4[(u_{\ell+1}^{(3)})^2 + (u_{\ell+2}^{(3)})^2]. \end{aligned} \quad (4.5)$$

We can now calculate explicitly the first equality below and then use (4.5) (with  $\mathbf{u}'$  replaced by  $\mathbf{u}''$ ) for the second equality to obtain

$$\begin{aligned}
(u'_\ell + u'_{\ell+1} + u'_{\ell+2} + u'_{\ell+3})^2 &= 4((u'_\ell)^2 + (u'_{\ell+1})^2 + (u'_{\ell+2})^2 + (u'_{\ell+3})^2) \\
&\quad - \epsilon^2 (u''_{\ell+1})^2 - \epsilon^2 (u''_{\ell+2})^2 - \epsilon^2 (u''_{\ell+3})^2 - \epsilon^2 (u''_{\ell+1} + u''_{\ell+2})^2 \\
&\quad - \epsilon^2 (u''_{\ell+2} + u''_{\ell+3})^2 - \epsilon^2 (u''_{\ell+1} + u''_{\ell+2} + u''_{\ell+3})^2 \\
&= 4((u'_\ell)^2 + (u'_{\ell+1})^2 + (u'_{\ell+2})^2 + (u'_{\ell+3})^2) \\
&\quad - \epsilon^2 (6(u''_{\ell+1})^2 + 8(u''_{\ell+2})^2 + 6(u''_{\ell+3})^2) \\
&\quad + \epsilon^4 (4(u_{\ell+2}^{(3)})^2 + 4(u_{\ell+3}^{(3)})^2) - \epsilon^6 (u_{\ell+3}^{(4)})^2.
\end{aligned}$$

We can then obtain from the above identities that

$$\begin{aligned}
\langle \delta^2 \hat{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle &= G_F'' \cdot \left\{ \left[ 4(\rho_F')^2 + 16(\rho_{2F}')^2 + 16\rho_F' \rho_{2F}' \right] \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \right. \\
&\quad - \epsilon^2 \left[ (\rho_F')^2 + 20(\rho_{2F}')^2 + 12\rho_F' \rho_{2F}' \right] \|D^{(2)}\mathbf{u}\|_{\ell_\epsilon^2}^2 \\
&\quad \left. + \epsilon^4 \left[ 8(\rho_{2F}')^2 + 2\rho_F' \rho_{2F}' \right] \|D^{(3)}\mathbf{u}\|_{\ell_\epsilon^2}^2 - \epsilon^6 (\rho_{2F}')^2 \|D^{(4)}\mathbf{u}\|_{\ell_\epsilon^2}^2 \right\} \\
&\quad + G_F' \cdot \left\{ (2\rho_F'' + 8\rho_{2F}'') \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 - 2\epsilon^2 \rho_{2F}'' \|D^{(2)}\mathbf{u}\|_{\ell_\epsilon^2}^2 \right\} \\
&= \left\{ 4G_F'' (\rho_F' + 2\rho_{2F}')^2 + 2G_F' (\rho_F'' + 4\rho_{2F}'') \right\} \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \\
&\quad - \epsilon^2 \left\{ G_F'' \left[ (\rho_F')^2 + 20(\rho_{2F}')^2 + 12\rho_F' \rho_{2F}' \right] + G_F' 2\rho_{2F}'' \right\} \|D^{(2)}\mathbf{u}\|_{\ell_\epsilon^2}^2 \\
&\quad + \epsilon^4 G_F'' \left[ 8(\rho_{2F}')^2 + 2\rho_F' \rho_{2F}' \right] \|D^{(3)}\mathbf{u}\|_{\ell_\epsilon^2}^2 \\
&\quad - \epsilon^6 G_F'' (\rho_{2F}')^2 \|D^{(4)}\mathbf{u}\|_{\ell_\epsilon^2}^2.
\end{aligned} \tag{4.6}$$

We define the *continuum elastic modulus for the embedding energy* to be

$$\hat{A}_F := 4G_F'' (\rho_F' + 2\rho_{2F}')^2 + 2G_F' (\rho_F'' + 4\rho_{2F}''). \tag{4.7}$$

and

$$\begin{aligned}
A_F &:= \hat{A}_F + \tilde{A}_F, \quad B_F := -[\phi_{2F}'' + G_F''((\rho_F')^2 + 20(\rho_{2F}')^2 + 12\rho_F' \rho_{2F}') + G_F' (2\rho_{2F}'')], \\
C_F &:= G_F'' (8(\rho_{2F}')^2 + 2\rho_F' \rho_{2F}'), \quad \text{and} \quad D_F := -G_F'' (\rho_{2F}')^2.
\end{aligned}$$

Then (4.1) becomes

$$\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle = A_F \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 + \epsilon^2 B_F \|D^{(2)}\mathbf{u}\|_{\ell_\epsilon^2}^2 + \epsilon^4 C_F \|D^{(3)}\mathbf{u}\|_{\ell_\epsilon^2}^2 + \epsilon^6 D_F \|D^{(4)}\mathbf{u}\|_{\ell_\epsilon^2}^2. \tag{4.8}$$

We will analyze the stability of  $\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  by using the Fourier representation [13]

$$Du_\ell = \sum_{k=-N+1}^N \frac{c_k}{\sqrt{2}} \cdot \exp\left(i k \frac{\ell}{N} \pi\right).$$



It then follows from the discrete orthogonality of the Fourier basis that

$$\begin{aligned} \langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle &= \sum_{k=-N+1}^N |c_k|^2 \cdot \left\{ A_F + B_F \left[ 4 \sin^2 \left( \frac{k\pi}{2N} \right) \right] \right. \\ &\quad \left. + C_F \left[ 4 \sin^2 \left( \frac{k\pi}{2N} \right) \right]^2 + D_F \left[ 4 \sin^2 \left( \frac{k\pi}{2N} \right) \right]^3 \right\}. \end{aligned} \quad (4.9)$$

We then see from (4.9) that the eigenvalues  $\lambda_k$  for  $k = -N+1, \dots, N$  of  $\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  with respect to the  $\|D\mathbf{u}\|_{\ell_\epsilon^2}$  norm are given by

$$\lambda_k = \lambda_F(s_k) \quad \text{for} \quad s_k = 4 \sin^2 \left( \frac{k\pi}{2N} \right)$$

where

$$\lambda_F(s) := A_F + B_F s + C_F s^2 + D_F s^3.$$

From the pair interaction potential, electron density function, and embedding energy function given in Figure 2 in [12], we assume that

$$\phi_F'' > 0, \phi_{2F}'' < 0; \quad \rho_F' \leq 0, \rho_{2F}' \leq 0; \quad \rho_F'' \geq 0, \rho_{2F}'' \geq 0; \quad \text{and} \quad G_F'' \geq 0. \quad (4.10)$$

We then have from the assumption (4.10) that

$$C_F > 0, \quad D_F < 0, \quad \text{and} \quad 8|D_F| \leq C_F. \quad (4.11)$$

We can check that (4.11) implies that  $|D_F s| \leq 4|D_F| \leq C_F/2$ , for  $0 \leq s \leq 4$ , so

$$\lambda_F'(s) = B_F + 2C_F s + 3D_F s^2 \geq B_F + \frac{C_F}{2} s \quad \text{for all} \quad 0 \leq s \leq 4. \quad (4.12)$$

We conclude from (4.12) that the condition  $B_F \geq 0$  or equivalently

$$\phi_{2F}'' + G_F'' \left[ (\rho_F')^2 + 20(\rho_{2F}')^2 + 12\rho_F' \rho_{2F}' \right] + G_F' 2\rho_{2F}'' = -B_F \leq 0, \quad (4.13)$$

and the assumptions (4.10) imply that  $\lambda(s)$  is increasing for  $0 \leq s \leq 4$ . We thus have the sharp stability result

$$\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle \geq \lambda_F(s_1) \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \geq (\hat{A}_F + \tilde{A}_F) \|D\mathbf{u}\|_{\ell_\epsilon^2}^2 \quad \text{for all} \quad \mathbf{u} \in \mathcal{U}. \quad (4.14)$$

We summarize this result in the following theorem:

**Theorem 4.1.** *Suppose that the hypotheses (4.10) and (4.13) hold. Then the uniform deformation  $\mathbf{y}_F$  is stable for the atomistic model if and only if*

$$\begin{aligned} \lambda_F(s_1) &= A_F + B_F \left[ 4 \sin^2 \left( \frac{\pi}{2N} \right) \right] + C_F \left[ 4 \sin^2 \left( \frac{\pi}{2N} \right) \right]^2 + D_F \left[ 4 \sin^2 \left( \frac{\pi}{2N} \right) \right]^3 \\ &= \hat{A}_F + \tilde{A}_F - 4 \sin^2 \left( \frac{\pi}{2N} \right) \left\{ \phi_{2F}'' + G_F'' \left[ (\rho_F')^2 + 20(\rho_{2F}')^2 + 12\rho_F' \rho_{2F}' \right] + G_F' 2\rho_{2F}'' \right\} \\ &\quad + 4^2 \sin^4 \left( \frac{\pi}{2N} \right) G_F'' \left[ \eta(\rho_{2F}')^2 + 2\rho_F' \rho_{2F}' \right] - 4^3 \sin^6 \left( \frac{\pi}{2N} \right) G_F'' (\rho_{2F}')^2 > 0. \end{aligned}$$

*Remark 4.1.* The role of the assumption (4.13) is to guarantee that  $u'_\ell = \sin(\epsilon\ell\pi)$  is the eigenfunction corresponding to the smallest eigenvalue of  $\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  with respect to the norm  $\|D\mathbf{u}\|_{\ell_\epsilon^2}$ . In fact, we can see from the above Fourier analysis that  $u'_\ell = \sin(\epsilon\ell\pi)$  is not the smallest eigenvalue of  $\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  with respect to the norm  $\|D\mathbf{u}\|_{\ell_\epsilon^2}$  for sufficiently large  $N$  if (4.13) does not hold since then  $\lambda'(0) < 0$ .

The assumption (4.13) on the the pair interaction potential, electron density function, and embedding energy function cannot be expected to generally hold for physical embedded atom models since the nearest neighbor term  $G_F''(\rho_F')^2 > 0$  dominates. We note, however, that generally  $G_F' < 0$  for  $F > 1$  [20], in which case  $G_F' 2\rho_{2F}'' < 0$ ; so (4.13) is more likely to hold for tensile strains  $F > 1$ .

**4.2. The EAM-QNL Model.** Now we will analyze the stability of the EAM-QNL model for next-nearest neighbor interactions. The Fourier techniques used to analyze the stability of the atomistic model cannot be used for the EAM-QNL model because the Fourier modes are no longer eigenfunctions. Recall that the total atomistic interaction energy of the QNL model is  $\mathcal{E}^{qnl}(\mathbf{y}) := \hat{\mathcal{E}}^{qnl}(\mathbf{y}) + \tilde{\mathcal{E}}^{qnl}(\mathbf{y}) = \epsilon \sum_{\ell=-N+1}^N \mathcal{E}_\ell^{qnl}(\mathbf{y})$ , where  $\mathcal{E}_\ell^{qnl}(\mathbf{y})$  is symmetric in  $\ell \in \{-N+1, \dots, N\}$  and is given by

$$\mathcal{E}_\ell^{qnl}(\mathbf{y}) := \begin{cases} \mathcal{E}_\ell^a(\mathbf{y}) & \text{for } 0 \leq \ell < K+1, \\ \mathcal{E}_{K+1}^{qnl}(\mathbf{y}) & \text{for } \ell = K+1, \\ \mathcal{E}_{K+2}^{qnl}(\mathbf{y}) & \text{for } \ell = K+2, \\ \mathcal{E}_\ell^c(\mathbf{y}) & \text{for } K+2 < \ell < N. \end{cases}$$

Since the QNL energy is consistent (see the consistency error analysis in Section 5),  $\mathbf{y}_F$  is still an equilibrium of  $\mathcal{E}^{qnl}(\mathbf{y})$  [25]. Therefore, we will focus on  $\langle \delta^2 \mathcal{E}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  to estimate the stability. The second variation of  $\mathcal{E}^{qnl}(\mathbf{y})$  evaluated at  $\mathbf{y} = \mathbf{y}_F$  is given by

$$\langle \delta^2 \mathcal{E}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle = \langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle + \langle \delta^2 \tilde{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle. \quad (4.15)$$

We first compute the second term of (4.15) and get

$$\begin{aligned} & \langle \delta^2 \tilde{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle \\ &= \epsilon \sum_{\ell=-K}^K \frac{1}{2} \left\{ \phi_F'' \left[ (u'_\ell)^2 + (u'_{\ell+1})^2 \right] + \phi_{2F}'' \left[ (u'_\ell + u'_{\ell-1})^2 + (u'_{\ell+1} + u'_{\ell+2})^2 \right] \right\} \\ & \quad + \frac{\epsilon}{2} \left\{ \phi_F'' \left[ (u'_{K+1})^2 + (u'_{K+2})^2 \right] + \phi_{2F}'' \left[ (u'_{K+1} + u'_K)^2 + 4(u'_{K+2})^2 \right] \right\} \\ & \quad + \frac{\epsilon}{2} \left\{ \phi_F'' \left[ (u'_{K+2})^2 + (u'_{K+3})^2 \right] + \phi_{2F}'' \left[ (u'_{K+2} + u'_{K+1})^2 + 4(u'_{K+3})^2 \right] \right\} \\ & \quad + \dots + \epsilon \sum_{\ell=K+3}^N \frac{1}{2} \left\{ \phi_F'' \left[ (u'_\ell)^2 + (u'_{\ell+1})^2 \right] + \phi_{2F}'' \left[ 4(u'_\ell)^2 + 4(u'_{\ell+1})^2 \right] \right\}. \end{aligned} \quad (4.16)$$

Here we omit the terms whose indices  $\ell \in \{-N+1, \dots, -(K+3)\}$  since the QNL energy is symmetric. Then we compute the first term, which is given by the following expression:

$$\begin{aligned}
\langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle = & \dots \\
& + \epsilon \sum_{\ell=0}^K \left\{ G_F'' [\rho_F'(u'_\ell + u'_{\ell+1}) + \rho_{2F}'(u'_{\ell-1} + u'_\ell + u'_{\ell+1} + u'_{\ell+2})]^2 \right. \\
& + G_F' [\rho_F''(u'_\ell)^2 + \rho_{2F}''(u'_\ell + u'_{\ell-1})^2 + \rho_F''(u'_{\ell+1})^2 + \rho_{2F}''(u'_{\ell+1} + u'_{\ell+2})^2] \left. \right\} \\
& + 2\epsilon G_F'' [\rho_F' u'_{K+1} + \rho_{2F}'(u'_{K+1} + u'_K)]^2 + \epsilon G_F' [\rho_F''(u'_{K+1})^2 + \rho_{2F}''(u'_{K+1} + u'_K)^2] \\
& + 2\epsilon G_F'' (\rho_F' + 2\rho_{2F}')^2 (u'_{K+2})^2 + \epsilon G_F' (\rho_F'' + 4\rho_{2F}'') (u'_{K+2})^2 \\
& + 2\epsilon G_F'' [\rho_F' u'_{K+2} + \rho_{2F}'(u'_{K+2} + u'_{K+1})]^2 + \epsilon G_F' [\rho_F''(u'_{K+2})^2 + \rho_{2F}''(u'_{K+2} + u'_{K+1})^2] \\
& + 2\epsilon G_F'' (\rho_F' + 2\rho_{2F}')^2 (u'_{K+3})^2 + \epsilon G_F' (\rho_F'' + 4\rho_{2F}'') (u'_{K+3})^2 \\
& + \epsilon \sum_{\ell=K+3}^N \left[ 2G_F'' (\rho_F' + 2\rho_{2F}')^2 + G_F' (\rho_F'' + 4\rho_{2F}'') \right] [(u'_\ell)^2 + (u'_{\ell+1})^2].
\end{aligned} \tag{4.17}$$

Now we use (4.5) again to rewrite (4.17) in the following form

$$\begin{aligned}
\langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle = & \epsilon \sum_{\ell=-N+1}^N \left[ 2G_F'' (\rho_F' + 2\rho_{2F}')^2 + G_F' (\rho_F'' + 4\rho_{2F}'') \right] [(u'_\ell)^2 + (u'_{\ell+1})^2] \\
& + \dots - \epsilon^3 \sum_{\ell=0}^K \left\{ G_F'' \cdot [(\rho_F')^2 + 20(\rho_{2F}')^2 + 12\rho_F' \rho_{2F}'] + G_F' \cdot 2\rho_{2F}'' \right\} \left( D^{(2)} u_\ell \right)^2 \\
& - \epsilon^3 \left\{ G_F'' \cdot [(\rho_F')^2 + 16(\rho_{2F}')^2 + 11\rho_F' \rho_{2F}'] + G_F' \cdot 2\rho_{2F}'' \right\} \left( D^{(2)} u_{K+1} \right)^2 \\
& - \epsilon^3 \left\{ G_F'' \cdot [8(\rho_{2F}')^2 + 5\rho_F' \rho_{2F}'] + G_F' \cdot 2\rho_{2F}'' \right\} \left( D^{(2)} u_{K+2} \right)^2 \\
& + \epsilon^5 \sum_{\ell=0}^{K+1} G_F'' \cdot [8(\rho_{2F}')^2 + 2\rho_F' \rho_{2F}'] \left( D^{(3)} u_\ell \right)^2 \\
& + \epsilon^5 G_F'' \cdot [4(\rho_{2F}')^2 + \rho_F' \rho_{2F}'] \left( D^{(3)} u_{K+2} \right)^2 - \epsilon^7 \sum_{\ell=0}^{K+2} G_F'' \cdot (\rho_{2F}')^2 \left( D^{(4)} u_\ell \right)^2.
\end{aligned}$$

Combining  $\langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  and  $\langle \delta^2 \tilde{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  together we obtain

$$\begin{aligned} \langle \delta^2 \mathcal{E}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle &= \epsilon \sum_{\ell=-N+1}^N \left( \hat{A}_F + \tilde{A}_F \right) (Du_\ell)^2 + \dots \\ &\quad - \epsilon^3 \sum_{\ell=0}^K \left\{ \phi_{2F}'' + G_F'' \cdot [(\rho_F')^2 + 20(\rho_{2F}')^2 + 12\rho_F' \rho_{2F}'] + G_F' \cdot 2\rho_{2F}'' \right\} \left( D^{(2)} u_\ell \right)^2 \\ &\quad - \epsilon^3 \left\{ \phi_{2F}'' + G_F'' \cdot [(\rho_F')^2 + 16(\rho_{2F}')^2 + 11\rho_F' \rho_{2F}'] + G_F' \cdot 2\rho_{2F}'' \right\} \left( D^{(2)} u_{K+1} \right)^2 \\ &\quad - \epsilon^3 \left\{ \phi_{2F}'' + G_F'' \cdot [8(\rho_{2F}')^2 + 5\rho_F' \rho_{2F}'] + G_F' \cdot 2\rho_{2F}'' \right\} \left( D^{(2)} u_{K+2} \right)^2 \\ &\quad + \epsilon^5 \sum_{\ell=0}^{K+1} G_F'' \cdot [8(\rho_{2F}')^2 + 2\rho_F' \rho_{2F}'] \left( D^{(3)} u_\ell \right)^2 \\ &\quad + \epsilon^5 G_F'' \cdot [4(\rho_{2F}')^2 + \rho_F' \rho_{2F}'] \left( D^{(3)} u_{K+2} \right)^2 - \epsilon^7 \sum_{\ell=0}^{K+2} G_F'' \cdot (\rho_{2F}')^2 \left( D^{(4)} u_\ell \right)^2. \end{aligned}$$

Because of the hypotheses (4.10) and (4.13), we have that

$$\begin{aligned} \phi_{2F}'' + G_F'' \cdot [(\rho_F')^2 + 16(\rho_{2F}')^2 + 11\rho_F' \rho_{2F}'] + G_F' \cdot 2\rho_{2F}'' &\leq 0, \\ \phi_{2F}'' + G_F'' \cdot [8(\rho_{2F}')^2 + 5\rho_F' \rho_{2F}'] + G_F' \cdot 2\rho_{2F}'' &\leq 0. \end{aligned}$$

Thus, using

$$\left( D^{(4)} u_\ell \right)^2 = \left[ \frac{1}{\epsilon} \left( D^{(3)} u_\ell - D^{(3)} u_{\ell-1} \right) \right]^2 \leq \frac{2}{\epsilon^2} \left[ \left( D^{(3)} u_\ell \right)^2 + \left( D^{(3)} u_{\ell-1} \right)^2 \right]$$

and noting that  $G_F'' \cdot (\rho_{2F}')^2 \geq 0$ , we have

$$\begin{aligned} &\epsilon^5 \sum_{\ell=0}^{K+1} G_F'' \cdot [8(\rho_{2F}')^2 + 2\rho_F' \rho_{2F}'] \left( D^{(3)} u_\ell \right)^2 \\ &\quad + \epsilon^5 G_F'' \cdot [4(\rho_{2F}')^2 + \rho_F' \rho_{2F}'] \left( D^{(3)} u_{K+2} \right)^2 - \epsilon^7 \sum_{\ell=0}^{K+2} G_F'' \cdot (\rho_{2F}')^2 \left( D^{(4)} u_\ell \right)^2 \\ &\geq \epsilon^5 \sum_{\ell=0}^{K+1} G_F'' \cdot [4(\rho_{2F}')^2 + 2\rho_F' \rho_{2F}'] \left( D^{(3)} u_\ell \right)^2 \\ &\quad + \epsilon^5 G_F'' \cdot [2(\rho_{2F}')^2 + \rho_F' \rho_{2F}'] \left( D^{(3)} u_{K+2} \right)^2 \geq 0. \end{aligned} \tag{4.18}$$

So, except in the case  $K \in \{N-2, \dots, N\}$  when there is no continuum region, it follows that  $\mathbf{y}_F$  is stable in the QNL model if and only if  $\hat{A}_F + \tilde{A}_F > 0$ .

Now we can give a sharp stability estimate for the QNL model from the above estimates and the arguments in [9, 15].

**Theorem 4.2.** *Suppose that  $K < N - 2$  and the hypotheses (4.10) and (4.13) hold, then the uniform deformation  $\mathbf{y}_F$  is stable in the QNL model if and only if  $\hat{A}_F + \tilde{A}_F > 0$ .*

*Remark 4.2.* The role of the assumption (4.13) in Theorem 4.2, as in Theorem 4.1, is to give a necessary condition for  $u'_\ell = \sin(\epsilon\ell\pi)$  to be the eigenfunction corresponding to the smallest eigenvalue of  $\langle \delta^2 \mathcal{E}^{qnl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  with respect to the norm  $\|D\mathbf{u}\|_{\ell_\epsilon^2}$ .

*Remark 4.3.* From Theorem 4.1 and Theorem 4.2, we conclude that the difference between the sharp stability conditions of the fully atomistic and QNL models is of order  $O(\epsilon^2)$ . This result is the same as for the pair potential case [7].

*Remark 4.4.* We noted in Remark 4.1 that the assumption (4.13) is necessary for Theorem 4.1. We now give an explicit example showing that the uniform deformation can be more stable for the EAM-QCL model than for the fully atomistic model when (4.13) fails. We recall that the EAM-QCL model is the EAM-QNL model with no atomistic region, that is,

$$\mathcal{E}^{qcl}(\mathbf{y}) := \epsilon \sum_{\ell=-N+1}^N \mathcal{E}_\ell^c(\mathbf{y}).$$

We consider the case when

$$\phi_{2F}'' + G_F'' (\rho_F' + 2\rho_{2F}')^2 + G_F' 2\rho_{2F}'' > 0, \quad (4.19)$$

which implies that (4.13) does not hold since it then follows from (4.10) that

$$\begin{aligned} & \phi_{2F}'' + G_F'' \left[ (\rho_F')^2 + 20 (\rho_{2F}')^2 + 12 \rho_F' \rho_{2F}' \right] + G_F' 2\rho_{2F}'' \\ &= \left[ \phi_{2F}'' + G_F'' (\rho_F' + 2\rho_{2F}')^2 + G_F' 2\rho_{2F}'' \right] + 8G_F'' \left( 2 (\rho_{2F}')^2 + \rho_F' \rho_{2F}' \right) \\ &> 0. \end{aligned}$$

We define the oscillatory displacement  $\tilde{\mathbf{u}}$  by

$$\tilde{u}_\ell = (-1)^\ell \epsilon / (2\sqrt{2}),$$

so

$$\tilde{u}'_\ell = (-1)^\ell / (\sqrt{2}), \quad \|D\tilde{\mathbf{u}}\|_{\ell_\epsilon^2} = 1, \quad \tilde{u}''_\ell = (-1)^\ell (\sqrt{2}) / \epsilon.$$

We then calculate from (4.2) and (4.4) that

$$\begin{aligned} \langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \tilde{\mathbf{u}}, \tilde{\mathbf{u}} \rangle &= \langle \delta^2 \tilde{\mathcal{E}}^a(\mathbf{y}_F) \tilde{\mathbf{u}}, \tilde{\mathbf{u}} \rangle + \langle \delta^2 \tilde{\mathcal{E}}^a(\mathbf{y}_F) \tilde{\mathbf{u}}, \tilde{\mathbf{u}} \rangle \\ &= \epsilon \sum_{\ell=-N+1}^N G_F' 2\rho_F'' \frac{1}{2} + (\phi_F'' + 4\phi_{2F}'') \|D\tilde{\mathbf{u}}\|_{\ell_\epsilon^2}^2 + (-\epsilon^2 \phi_{2F}'') \|D^{(2)} \tilde{\mathbf{u}}\|_{\ell_\epsilon^2}^2 \\ &= G_F' 2\rho_F'' + (\phi_F'' + 4\phi_{2F}'') - 4\phi_{2F}'' = \phi_F'' + G_F' 2\rho_F''. \end{aligned} \quad (4.20)$$

Thus, we obtain that

$$\inf_{\mathbf{u} \in \mathcal{U} \setminus \{\mathbf{0}\}, \|D\mathbf{u}\|_{\ell_\epsilon^2} = 1} \langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle \leq \phi_F'' + G_F' 2\rho_F''.$$

On the other hand, we have that

$$\inf_{\mathbf{u} \in \mathcal{U} \setminus \{\mathbf{0}\}, \|D\mathbf{u}\|_{\ell_\epsilon^2} = 1} \langle \delta^2 \mathcal{E}^{qcl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle = \tilde{A}_F + \tilde{A}_F = 4 \left[ \phi_{2F}'' + G_F'' (\rho_F' + 2\rho_{2F}')^2 + G_F' 2\rho_{2F}'' \right] + \phi_F'' + G_F' 2\rho_F''.$$

Therefore, from (4.19) we have

$$\inf_{\mathbf{u} \in \mathcal{U} \setminus \{\mathbf{0}\}, \|D\mathbf{u}\|_{\ell_\epsilon^2} = 1} \langle \delta^2 \mathcal{E}^{qcl}(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle > \phi_F'' + G_F' 2\rho_F'' \geq \inf_{\mathbf{u} \in \mathcal{U} \setminus \{\mathbf{0}\}, \|D\mathbf{u}\|_{\ell_\epsilon^2} = 1} \langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle.$$

This inequality indicates that the uniform deformation  $\mathbf{y}_F$  can be unstable for the atomistic model, but stable for the EAM-QCL model, when the assumption (4.19) fails.

We cannot conclude from this argument, though, that the atomistic model is less stable than the EAM-QNL model with a nontrivial atomistic region, i.e.,  $K > 0$ . To see this, we consider an oscillatory displacement  $\hat{\mathbf{u}} \in \mathcal{U}$  with support only in the atomistic region (a similar test function is used in [2]):

$$\hat{u}_\ell = \begin{cases} \frac{(-1)^\ell \epsilon}{2\sqrt{2}}, & \ell = -(K-1), \dots, (K-1), \\ 0, & \text{otherwise.} \end{cases}$$

Then since  $\hat{u}'_\ell = (\hat{u}_\ell - \hat{u}_{\ell-1})/\epsilon$ , we have

$$\hat{u}'_\ell = \begin{cases} \frac{(-1)^\ell}{\sqrt{2}}, & \ell = -(K-2), \dots, (K-1), \\ \frac{(-1)^K}{2\sqrt{2}}, & \ell = K, \\ \frac{(-1)^{-(K-1)}}{2\sqrt{2}}, & \ell = -(K-1), \\ 0, & \text{otherwise.} \end{cases}$$

We substitute the displacement  $\hat{\mathbf{u}}$  into (4.17) and get

$$\begin{aligned} \langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \hat{\mathbf{u}}, \hat{\mathbf{u}} \rangle &= \epsilon \sum_{\ell=-(K-2)}^{K-3} G'_F \rho''_F + 2\epsilon \left\{ G''_F \frac{1}{8} \left[ 3(\rho'_{2F})^2 + 2(\rho'_F - \rho'_{2F})^2 \right] + G'_F \left[ \frac{7}{4} \rho''_F + \frac{1}{2} \rho''_{2F} \right] \right\} \\ &= \epsilon 2(K-2) G'_F \rho''_F + O(\epsilon). \end{aligned} \quad (4.21)$$

Similarly, we substitute  $\hat{\mathbf{u}}$  into (4.16) and get

$$\langle \delta^2 \tilde{\mathcal{E}}^{qnl}(\mathbf{y}_F) \hat{\mathbf{u}}, \hat{\mathbf{u}} \rangle = \epsilon \sum_{\ell=-(K-2)}^{K-3} \frac{1}{2} \phi''_F + O(\epsilon) = \epsilon(K-2) \phi''_F + O(\epsilon). \quad (4.22)$$

Therefore, we obtain that

$$\langle \delta^2 \mathcal{E}^{qnl}(\mathbf{y}_F) \hat{\mathbf{u}}, \hat{\mathbf{u}} \rangle = \langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \hat{\mathbf{u}}, \hat{\mathbf{u}} \rangle + \langle \delta^2 \tilde{\mathcal{E}}^{qnl}(\mathbf{y}_F) \hat{\mathbf{u}}, \hat{\mathbf{u}} \rangle = \epsilon(K-2)(\phi''_F + 2G'_F \rho''_F) + O(\epsilon).$$

Note that

$$\|\hat{\mathbf{u}}'\|_{\ell^2_\epsilon}^2 = \epsilon \sum_{\ell=-N+1}^N (u'_\ell)^2 = \epsilon(K-1) + \frac{\epsilon}{4},$$

Thus, we obtain from the above and (4.20) that

$$\frac{\langle \delta^2 \mathcal{E}^{qnl}(\mathbf{y}_F) \hat{\mathbf{u}}, \hat{\mathbf{u}} \rangle}{\|\hat{\mathbf{u}}'\|_{\ell^2_\epsilon}^2} = (\phi''_F + 2G'_F \rho''_F) + O\left(\frac{1}{K}\right) = \frac{\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \tilde{\mathbf{u}}, \tilde{\mathbf{u}} \rangle}{\|\tilde{\mathbf{u}}'\|_{\ell^2_\epsilon}^2} + O\left(\frac{1}{K}\right).$$

This indicates that when (4.19) holds and  $K$  is sufficiently large, the EAM-QNL model is also less stable than the EAM-QCL model.

## 5. CONSISTENCY ERROR AND CONVERGENCE OF THE EAM-QNL MODEL.

Setting  $\mathbf{y}^{qnl} = \mathbf{y}_F + \mathbf{u}^{qnl}$  and  $\mathbf{y}^a = \mathbf{y}_F + \mathbf{u}^a$ , where both  $\mathbf{u}^{qnl}$  and  $\mathbf{u}^a$  belong to  $\mathcal{U}$ , we define the quasicontinuum error to be

$$\mathbf{e}^{qnl} := \mathbf{y}^a - \mathbf{y}^{qnl} = \mathbf{u}^a - \mathbf{u}^{qnl}.$$

To simplify the error analysis, we consider the linearization of the atomistic equilibrium equations (3.3) and the associated EAM-QNL equilibrium equations (3.5) about the uniform deformation  $\mathbf{y}_F$ . The linearized atomistic equation is

$$-\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle = \langle \delta \mathcal{F}(\mathbf{y}_F), \mathbf{w} \rangle \quad \text{for all } \mathbf{w} \in \mathcal{U}, \quad (5.1)$$

and the linearized EAM-QNL equation is

$$-\langle \delta^2 \mathcal{E}^{qnl}(\mathbf{y}_F) \mathbf{u}^{qnl}, \mathbf{w} \rangle = \langle \delta \mathcal{F}(\mathbf{y}_F), \mathbf{w} \rangle \quad \text{for all } \mathbf{w} \in \mathcal{U}. \quad (5.2)$$

We thus analyze the linearized error equation

$$\langle \delta^2 \mathcal{E}^{qnl}(\mathbf{y}_F) \mathbf{e}^{qnl}, \mathbf{w} \rangle = \langle \mathbf{T}^{qnl}, \mathbf{w} \rangle \quad \text{for all } \mathbf{w} \in \mathcal{U}, \quad (5.3)$$

where the linearized consistency error is given by

$$\begin{aligned} \langle \mathbf{T}^{qnl}, \mathbf{w} \rangle &:= \langle \delta^2 \mathcal{E}^{qnl}(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle - \langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle \\ &= \langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle - \langle \delta^2 \hat{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle \\ &\quad + \langle \delta^2 \tilde{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle - \langle \delta^2 \tilde{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle. \end{aligned} \quad (5.4)$$

Now we will give an estimate of the consistency error  $\langle \mathbf{T}^{qnl}, \mathbf{w} \rangle$  in the following theorem. We first define

$$\|\mathbf{v}\|_{\ell_\epsilon^2(\mathcal{C})}^2 := \epsilon \sum_{\ell \in \mathcal{C}} v_\ell^2, \quad \|\mathbf{v}\|_{\ell_\epsilon^2(\mathcal{I})}^2 := \epsilon \sum_{\ell \in \mathcal{I}} v_\ell^2, \quad \text{and} \quad \|\mathbf{v}\|_{\ell_\epsilon^\infty(\mathcal{I})}^2 := \max_{\ell \in \mathcal{I}} |v_\ell|, \quad \text{for } \mathbf{v} \in \mathcal{U},$$

where  $\mathcal{C}$  denotes the continuum region  $\{-N+1, \dots, -(K+1)\} \cup \{K+1, \dots, N\}$  and  $\mathcal{I}$  denotes the interface  $\{-(K+7), \dots, -K\} \cup \{K, \dots, K+7\}$ .

**Theorem 5.1.** *The consistency error  $\langle \mathbf{T}^{qnl}, \mathbf{w} \rangle$ , given in (5.4), satisfies the following negative norm estimate*

$$\begin{aligned} \left| \langle \mathbf{T}^{qnl}, \mathbf{w} \rangle \right| &\leq \left\{ \epsilon^2 [G_F'' \cdot ((\rho_F')^2 + 12\rho_F' \rho_{2F}' + 20(\rho_{2F}')^2) - 2G_F' \cdot \rho_{2F}'' + |\phi_{2F}''|] \cdot \|D^{(3)} \mathbf{u}^a\|_{\ell_\epsilon^2(\mathcal{C})} \right. \\ &\quad \left. + \epsilon^{3/2} (C_1 + C_2) \|D^{(2)} \mathbf{u}^a\|_{\ell_\epsilon^\infty(\mathcal{I})} \right\} \|D\mathbf{w}\|_{\ell_\epsilon^2} \quad \text{for all } \mathbf{w} \in \mathcal{U}. \end{aligned}$$

**Proof** We focus on the first term of (5.4)

$$\langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle - \langle \delta^2 \hat{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle = \dots + \mathbf{I}_0 + \mathbf{I}_1 + \mathbf{I}_2 + \mathbf{I}_3,$$

where  $\mathbf{I}_0$  is associated with  $\ell = 0, \dots, K$ ,  $\mathbf{I}_1$  is associated with  $\ell = K+1$ ,  $\mathbf{I}_2$  is associated with  $\ell = K+2$  and  $\mathbf{I}_3$  is associated with  $\ell = K+3, \dots, N$ .

We first compute  $\mathbf{I}_3$ . Note that  $\mathbf{u}^a$  and  $\mathbf{w}$  are  $2N$ -periodic, so in the calculation, when the indices  $\ell + i > N, i = 1, 2$ , we can move these terms to the  $\{-N+1, \dots, -1\}$  part by using the periodicity

as done in (6.9) in [15]. Hence, we can rearrange the terms in  $\mathbf{I}_3$  to get

$$\begin{aligned}
\mathbf{I}_3 = & \epsilon \sum_{\ell=K+5}^N G_F'' \cdot (\rho_F')^2 (-Du_{\ell-1}^a + 2Du_{\ell}^a - Du_{\ell+1}^a) Dw_{\ell} \\
& + \epsilon \sum_{\ell=K+5}^N G_F'' \cdot (\rho_F' \rho_{2F}') [4(-Du_{\ell-1}^a + 2Du_{\ell}^a - Du_{\ell+1}^a) + 2(-Du_{\ell-2}^a + 2Du_{\ell}^a - Du_{\ell+2}^a)] Dw_{\ell} \\
& + \epsilon \sum_{\ell=K+5}^N G_F'' \cdot (\rho_{2F}')^2 [3(-Du_{\ell-1}^a + 2Du_{\ell}^a - Du_{\ell+1}^a) + 2(-Du_{\ell-2}^a + 2Du_{\ell}^a - Du_{\ell+2}^a) \\
& \quad + (-Du_{\ell-3}^a + 2Du_{\ell}^a - Du_{\ell+3}^a)] Dw_{\ell} \\
& + \epsilon \sum_{\ell=K+5}^N 2G_F' \cdot \rho_{2F}'' (-Du_{\ell-1}^a + 2Du_{\ell}^a - Du_{\ell+1}^a) Dw_{\ell} + \mathbf{I}_{31}
\end{aligned} \tag{5.5}$$

where  $\mathbf{I}_{31}$  consists of the interfacial terms, i.e.,  $\ell \in \{K, \dots, K+7\}$ , and is given by the following expression

$$\begin{aligned}
\mathbf{I}_{31} = & \epsilon G_F'' \{ (\rho_F')^2 [(Du_{K+3}^a - Du_{K+4}^a) w'_{K+3} + (-Du_{K+3}^a + 2Du_{K+4}^a - Du_{K+5}^a) w'_{K+4}] \\
& + \rho_F' \rho_{2F}' [- (Du_{K+3}^a + Du_{K+4}^a) w'_{K+2} + (6Du_{K+3}^a - Du_{K+2}^a - 3Du_{K+4}^a - 2Du_{K+5}^a) w'_{K+3} \\
& \quad + (12Du_{K+4}^a - Du_{K+2}^a - 3Du_{K+3}^a - 4Du_{K+5}^a - 2Du_{K+6}^a) w'_{K+4}] \\
& + (\rho_{2F}')^2 [- (Du_{K+2}^a + Du_{K+3}^a + Du_{K+4}^a + Du_{K+5}^a) w'_{K+2} \\
& \quad + (6Du_{K+3}^a - Du_{K+2}^a - 2Du_{K+4}^a - 2Du_{K+5}^a - Du_{K+6}^a) w'_{K+3} \\
& \quad + (13Du_{K+4}^a - Du_{K+2}^a - 2Du_{K+3}^a - 3Du_{K+5}^a - 2Du_{K+6}^a - Du_{K+7}^a) w'_{K+4}] \} \\
& + \epsilon G_F' \rho_{2F}'' \{ - (Du_{K+2}^a + Du_{K+3}^a) w'_{K+2} + (2Du_{K+3}^a - Du_{K+2}^a - Du_{K+4}^a) w'_{K+3} \\
& \quad + (5Du_{K+4}^a - Du_{K+3}^a - 2Du_{K+5}^a) w'_{K+4} \}.
\end{aligned}$$

Since  $\mathbf{I}_0$  is associated with  $\ell = 0, \dots, K$  where the QNL and the atomistic models coincide with each other, we have  $\mathbf{I}_0 = 0$ . Similarly, by direct computation we get the following expression for



the sum of  $\mathbf{I}_1$  and  $\mathbf{I}_2$

$$\begin{aligned}
\mathbf{I}_1 + \mathbf{I}_2 = & \epsilon G_F'' \{ (\rho_F')^2 [(Du_{K+1}^a - Du_{K+2}^a) (w'_{K+1} - w'_{K+2})] \\
& + \rho_F' \rho_{2F}' [(Du_{K+1}^a - Du_{K+2}^a) w'_K + (2Du_{K+1}^a - 2Du_{K+2}^a + Du_K^a - Du_{K+3}^a) w'_{K+1} \\
& + (6Du_{K+2}^a - Du_K^a - 2Du_{K+1}^a - Du_{K+3}^a) w'_{K+2} - (Du_{K+1}^a + Du_{K+2}^a) w'_{K+3}] \\
& + (\rho_{2F}')^2 [(Du_K^a + Du_{K+1}^a - Du_{K+2}^a - Du_{K+3}^a) (w'_K + w'_{K+1}) \\
& + (7Du_{K+2}^a - Du_K^a - Du_{K+1}^a - Du_{K+3}^a) w'_{K+2} \\
& - (Du_K^a + Du_{K+1}^a + Du_{K+2}^a + Du_{K+3}^a) w'_{K+3}] \} \\
& + \epsilon G_F' \rho_{2F}'' \{ (3Du_{K+2}^a - Du_{K+3}^a) w'_{K+2} - (Du_{K+2}^a + Du_{K+3}^a) w'_{K+3} \} \\
& + \epsilon G_F'' \{ (\rho_F')^2 [(Du_{K+2}^a - Du_{K+3}^a) (w'_{K+2} - w'_{K+3})] \\
& + \rho_F' \rho_{2F}' [(Du_{K+2}^a - Du_{K+3}^a) w'_{K+1} + (2Du_{K+2}^a - 2Du_{K+3}^a + Du_{K+1}^a - Du_{K+4}^a) w'_{K+2} \\
& + (6Du_{K+3}^a - Du_{K+1}^a - 2Du_{K+2}^a - Du_{K+4}^a) w'_{K+3} - (Du_{K+2}^a + Du_{K+3}^a) w'_{K+4}] \\
& + (\rho_{2F}')^2 [(Du_{K+1}^a + Du_{K+2}^a - Du_{K+3}^a - Du_{K+4}^a) (w'_{K+1} + w'_{K+2}) \\
& + (7Du_{K+3}^a - Du_{K+1}^a - Du_{K+2}^a - Du_{K+4}^a) w'_{K+3} \\
& - (Du_{K+1}^a + Du_{K+2}^a + Du_{K+3}^a + Du_{K+4}^a) w'_{K+4}] \} \\
& + \epsilon G_F' \rho_{2F}'' \{ (3Du_{K+3}^a - Du_{K+4}^a) w'_{K+3} - (Du_{K+3}^a + Du_{K+4}^a) w'_{K+4} \}.
\end{aligned} \tag{5.6}$$

Note that we can rewrite the second term of the second line of  $\mathbf{I}_3$  as

$$\begin{aligned}
2(-Du_{\ell-2}^a + 2Du_{\ell-1}^a - Du_{\ell+2}^a) &= 2(-Du_{\ell-2}^a + 2Du_{\ell-1}^a - Du_{\ell}^a) + 4(-Du_{\ell-1}^a + 2Du_{\ell}^a - Du_{\ell+1}^a) \\
&+ 2(-Du_{\ell}^a + 2Du_{\ell+1}^a - Du_{\ell+2}^a).
\end{aligned}$$

Similarly, we can rewrite the third term of the third line of  $\mathbf{I}_3$  as

$$\begin{aligned}
(-Du_{\ell-3}^a + 2Du_{\ell-2}^a - Du_{\ell+3}^a) &= (-Du_{\ell-3}^a + 2Du_{\ell-2}^a - Du_{\ell-1}^a) + 2(-Du_{\ell-2}^a + 2Du_{\ell-1}^a - Du_{\ell}^a) \\
&+ 3(-Du_{\ell-1}^a + 2Du_{\ell}^a - Du_{\ell+1}^a) + 2(-Du_{\ell}^a + 2Du_{\ell+1}^a - Du_{\ell+2}^a) \\
&+ (-Du_{\ell+1}^a + 2Du_{\ell+2}^a - Du_{\ell+3}^a).
\end{aligned}$$

Then we combine  $\mathbf{I}_1$ ,  $\mathbf{I}_2$  and  $\mathbf{I}_3$  together and rearrange the interfacial terms, i.e.,  $\ell \in \{K, \dots, K+7\}$ . We find that the coefficients of the interfacial terms  $\mathbf{I}_1 + \mathbf{I}_2 + \mathbf{I}_{31}$  are perfectly matched so that they are of order  $\epsilon$ , thus we obtain the following estimate by the Cauchy-Schwarz inequality:

$$\begin{aligned}
& \left| \langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle - \langle \delta^2 \hat{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle \right| \\
& \leq \left\{ [G_F'' \cdot ((\rho_F')^2 + 12\rho_F' \rho_{2F}' + 20(\rho_{2F}')^2) - 2G_F' \cdot \rho_{2F}''] \epsilon^2 \cdot \|D^{(3)} \mathbf{u}^a\|_{\ell_\epsilon^2(\mathcal{C})} \right. \\
& \quad \left. + C_1 \epsilon \cdot \|D^{(2)} \mathbf{u}^a\|_{\ell_\epsilon^2(\mathcal{I})} \right\} \|D \mathbf{w}\|_{\ell_\epsilon^2}
\end{aligned} \tag{5.7}$$

where  $\mathcal{I}$  is the interface:  $\{K, \dots, K+7\}$ , and  $C_1$  is a constant independent of  $\epsilon$ . We note that

$$\|D^2 \mathbf{u}^a\|_{\ell_\epsilon^2(\mathcal{I})}^2 = \epsilon \sum_{\ell=K}^{K+7} \left| D^{(2)} u_\ell^a \right|^2 \leq \|D^{(2)} \mathbf{u}^a\|_{\ell_\epsilon^\infty(\mathcal{I})}^2 \sum_{\ell=K}^{K+7} \epsilon = 8\epsilon \|D^{(2)} \mathbf{u}^a\|_{\ell_\epsilon^\infty(\mathcal{I})}^2.$$

Thus, we obtain

$$\begin{aligned} & \left| \langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle - \langle \delta^2 \hat{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle \right| \\ & \leq \left\{ \epsilon^2 [G_F'' \cdot ((\rho_F')^2 + 12\rho_F' \rho_{2F}' + 20(\rho_{2F}')^2) - 2G_F' \cdot \rho_{2F}''] \cdot \|D^{(3)} \mathbf{u}^a\|_{\ell_\epsilon^2(\mathcal{C})} \right. \\ & \quad \left. + \epsilon^{3/2} C_1 \|D^{(2)} \mathbf{u}^a\|_{\ell_\epsilon^\infty(\mathcal{I})} \right\} \cdot \|D\mathbf{w}\|_{\ell_\epsilon^2}. \end{aligned}$$

We can estimate the pair potential consistency error,  $\langle \delta^2 \tilde{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle - \langle \delta^2 \tilde{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle$ , by considering the above estimate for an embedding energy  $G(\tilde{\phi}) = \tilde{\phi}/2$  to obtain

$$\begin{aligned} & \left| \langle \delta^2 \tilde{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle - \langle \delta^2 \tilde{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle \right| \\ & \leq \left\{ \epsilon^2 |\phi_{2F}''| \|D^{(3)} \mathbf{u}\|_{\ell_\epsilon^2(\mathcal{C})} + C_2 \epsilon \|D^{(2)} \mathbf{u}^a\|_{\ell_\epsilon^2(\mathcal{I})} \right\} \|D\mathbf{w}\|_{\ell_\epsilon^2} \\ & \leq \left\{ \epsilon^2 |\phi_{2F}''| \|D^{(3)} \mathbf{u}\|_{\ell_\epsilon^2(\mathcal{C})} + C_2 \epsilon^{3/2} \|D^{(2)} \mathbf{u}^a\|_{\ell_\epsilon^\infty(\mathcal{I})} \right\} \|D\mathbf{w}\|_{\ell_\epsilon^2}. \end{aligned}$$

Therefore, we obtain the following optimal order estimate for the consistency error (5.4)

$$\begin{aligned} \left| \langle \mathbf{T}^{qnl}, \mathbf{w} \rangle \right| & \leq \left| \langle \delta^2 \hat{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle - \langle \delta^2 \hat{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle \right| \\ & \quad + \left| \langle \delta^2 \tilde{\mathcal{E}}^{qnl}(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle - \langle \delta^2 \tilde{\mathcal{E}}^a(\mathbf{y}_F) \mathbf{u}^a, \mathbf{w} \rangle \right| \\ & \leq \left\{ \epsilon^2 [G_F'' \cdot ((\rho_F')^2 + 12\rho_F' \rho_{2F}' + 20(\rho_{2F}')^2) - 2G_F' \cdot \rho_{2F}'' + |\phi_{2F}''|] \cdot \|D^{(3)} \mathbf{u}^a\|_{\ell_\epsilon^2(\mathcal{C})} \right. \\ & \quad \left. + \epsilon^{3/2} (C_1 + C_2) \|D^{(2)} \mathbf{u}^a\|_{\ell_\epsilon^\infty(\mathcal{I})} \right\} \|D\mathbf{w}\|_{\ell_\epsilon^2} \quad \text{for all } \mathbf{w} \in \mathcal{U}. \end{aligned}$$

□

We can now give the convergence result for the linearized EAM-QNL model.

**Theorem 5.2.** *Suppose that  $\hat{A}_F + \tilde{A}_F > 0$ , where  $\hat{A}_F$  and  $\tilde{A}_F$  are defined in (4.7) and (4.3), and that (4.10) and (4.13) holds. Then the linearized atomistic problem (5.1) as well as the linearized QNL approximation (5.2) have unique solutions, and they satisfy the error estimate*

$$\begin{aligned} \|D\mathbf{y}^a - D\mathbf{y}^{qnl}\|_{\ell_\epsilon^2} & = \|D\mathbf{u}^a - D\mathbf{u}^{qnl}\|_{\ell_\epsilon^2} \\ & \leq \frac{\epsilon^2 [G_F'' \cdot ((\rho_F')^2 + 12\rho_F' \rho_{2F}' + 20(\rho_{2F}')^2) - 2G_F' \cdot \rho_{2F}'' + |\phi_{2F}''|] \cdot \|D^{(3)} \mathbf{u}^a\|_{\ell_\epsilon^2(\mathcal{C})}}{\hat{A}_F + \tilde{A}_F} \\ & \quad + \frac{\epsilon^{3/2} (C_1 + C_2) \|D^{(2)} \mathbf{u}^a\|_{\ell_\epsilon^\infty(\mathcal{I})}}{\hat{A}_F + \tilde{A}_F}. \end{aligned}$$

**Proof.** The error estimate for the EAM-QNL model follows from the error equation (5.3), the stability estimate in Theorem 4.2, and the consistency estimate in Theorem 5.1. □

## 6. CONCLUSION.

We describe a one-dimensional QNL method for the EAM potential following [25], and we study the stability and convergence of a linearization of the next-nearest neighbor EAM-QNL energy. We identify conditions for the pair potential, electron density function, and embedding function so that the lattice stability of the atomistic and the EAM-QNL models are asymptotically equal. These condition are necessary to guarantee that  $u'_\ell = \sin(\epsilon\ell\pi)$  is the eigenfunction corresponding to the smallest eigenvalue of  $\langle \delta^2 \mathcal{E}^a(\mathbf{y}_F) \mathbf{u}, \mathbf{u} \rangle$  with respect to the norm  $\|D\mathbf{u}\|_{\ell_\epsilon^2}$ .

We then give a negative norm estimate for the consistency error and generalize the conclusions in [6] to the EAM case. We compare the equilibria of the atomistic and EAM-QNL models and give an optimal order  $O(\epsilon^{3/2})$  error estimate for the  $\ell_\epsilon^2$  norm of the strain in terms of the deformation in the continuum region.

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## REFERENCES

- [1] S. Badia, M. L. Parks, P. B. Bochev, M. Gunzburger, and R. B. Lehoucq. On atomistic-to-continuum coupling by blending. *SIAM J. Multiscale Modeling & Simulation*, 7(1):381–406, 2008.
- [2] P. Belik and M. Luskin. Sharp stability and optimal order error analysis of the quasi-nonlocal approximation of unconstrained linear and circular chains in 2-d. arXiv:1008.3716, 2010.
- [3] W. Curtin and R. Miller. Atomistic/continuum coupling in computational materials science. *Modell. Simul. Mater. Sci. Eng.*, 11(3):R33–R68, 2003.
- [4] M. Dobson and M. Luskin. Analysis of a force-based quasicontinuum approximation. *M2AN Math. Model. Numer. Anal.*, 42(1):113–139, 2008.
- [5] M. Dobson and M. Luskin. Iterative solution of the quasicontinuum equilibrium equations with continuation. *Journal of Scientific Computing*, 37:19–41, 2008.
- [6] M. Dobson and M. Luskin. An optimal order error analysis of the one-dimensional quasicontinuum approximation. *SIAM J. Numer. Anal.*, 47:2455–2475, 2009.
- [7] M. Dobson, M. Luskin, and C. Ortner. Sharp stability estimates for the force-based quasicontinuum approximation of homogeneous tensile deformation. *SIAM J. Multiscale Modeling & Simulation*, 8:782–802, 2010.
- [8] M. Dobson, M. Luskin, and C. Ortner. Stability, instability, and error of the force-based quasicontinuum approximation. *Archive for Rational Mechanics and Analysis*, 197:179–202, 2010.
- [9] M. Dobson, M. Luskin, and C. Ortner. Accuracy of quasicontinuum approximations near instabilities. *Journal of the Mechanics and Physics of Solids*, to appear.
- [10] M. Dobson, M. Luskin, and C. Ortner. Iterative methods for the force-based quasicontinuum approximation. *Computer Methods in Applied Mechanics and Engineering*, to appear. arXiv:0910.2013v3.
- [11] W. E, J. Lu, and J. Yang. Uniform accuracy of the quasicontinuum method. *Phys. Rev. B*, 74(21):214115, 2004.
- [12] S. M. Foiles, M. I. Baskes, and M. S. Daw. Embedded-atom-method functions for the fcc metals Cu, Ag, Au, Ni, Pd, Pt, and their alloys. *Phys. Rev. B*, 33:7983–7911, 1986.
- [13] T. Hudson and C. Ortner. On the stability of bravais lattices and their Cauchy–Born approximations. in preparation.
- [14] R. A. Johnson and D. J. Oh. Analytic embedded atom method model for bcc metals. *JMR.*, 4:1195–1201, 1989.
- [15] X. Li and M. Luskin. A generalized quasi-nonlocal atomistic-to-continuum coupling method with finite range interaction. arXiv:1007.2336, 2010.
- [16] P. Lin. Convergence analysis of a quasi-continuum approximation for a two-dimensional material without defects. *SIAM J. Numer. Anal.*, 45(1):313–332 (electronic), 2007.
- [17] R. Miller and E. Tadmor. The quasicontinuum method: overview, applications and current directions. *Journal of Computer-Aided Materials Design*, 9:203–239, 2003.
- [18] R. Miller and E. Tadmor. Benchmarking multiscale methods. *Modelling and Simulation in Materials Science and Engineering*, 17:053001 (51pp), 2009.
- [19] P. Ming and J. Z. Yang. Analysis of a one-dimensional nonlocal quasi-continuum method. *Multiscale Model. Simul.*, 7(4):1838–1875, 2009.
- [20] Y. Mishin, M. J. Mehl, D. A. Papaconstantopoulos, A. F. Voter, and J. D. Kress. Structural stability and lattice defects in copper: Ab initio, tight-binding, and embedded-atom calculations. *Phys. Rev. B*, 63, 2001.
- [21] M. Ortiz, R. Phillips, and E. B. Tadmor. Quasicontinuum analysis of defects in solids. *Philosophical Magazine A*, 73(6):1529–1563, 1996.
- [22] C. Ortner. A priori and a posteriori analysis of the quasi-nonlocal quasicontinuum method in 1D. *Math. Comp.*, to appear.
- [23] A. V. Shapeev. Consistent energy-based atomistic/continuum coupling for two-body potential: 1D and 2D case. preprint, 2010.

- [24] V. B. Shenoy, R. Miller, E. B. Tadmor, D. Rodney, R. Phillips, and M. Ortiz. An adaptive finite element approach to atomic-scale mechanics—the quasicontinuum method. *J. Mech. Phys. Solids*, 47(3):611–642, 1999.
- [25] T. Shimokawa, J. Mortensen, J. Schiotz, and K. Jacobsen. Matching conditions in the quasicontinuum method: Removal of the error introduced at the interface between the coarse-grained and fully atomistic region. *Phys. Rev. B*, 69(21):214104, 2004.